Fumaric acid, dipentafluorophenyl ester

Inchi: InChI=1S/C16H2F10O4/c17-5-7(19)11(23)15(12(24)8(5)20)29-3(27)1-2-4(28)30-16-13(2
InchiKey: FYFBDXSBTQNZDS-OWOJBTEDSA-N
Formula: C16H2F10O4
SMILES: O=C(C=CC(=O)Oc1c(F)c(F)c(F)c(F)c1F)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 448.17

Physical Properties

Property code	Value	Unit	Source
gf	-2123.36	kJ/mol	Joback Method
hf	-2348.69	kJ/mol	Joback Method
hfus	57.96	kJ/mol	Joback Method
hvap	72.48	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	4.145		Crippen Method
mcvol	217.060	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
rinpol	1763.00		NIST Webbook
tb	818.08	K	Joback Method
tc	1006.69	K	Joback Method
tf	593.26	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.88	J/mol×K	818.08	Joback Method
cpg	603.00	J/mol×K	849.51	Joback Method
cpg	610.45	J/mol×K	880.95	Joback Method
cpg	617.22	J/mol×K	912.38	Joback Method
cpg	623.32	J/mol×K	943.82	Joback Method
cpg	628.72	J/mol×K	975.25	Joback Method
cpg	633.43	J/mol×K	1006.69	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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